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(Statement A)

Polynitrogen Chemistry

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Under combined DARPA, AFOSR, NSF, and DOE sponsorship, we have continued our work in polynitrogen chemistry. We have successfully prepared and characterized numerous polyazido compounds, such as $\text{As}(\text{N}_3)_3$, $\text{Sb}(\text{N}_3)_3$, $\text{As}(\text{N}_3)_5$, $\text{Sb}(\text{N}_3)_5$, $\text{As}(\text{N}_3)_6^-$, $\text{Sb}(\text{N}_3)_6^-$, $\text{Te}(\text{N}_3)_4$, $\text{Te}(\text{N}_3)_6^{2-}$, $\text{P}(\text{N}_3)_6^-$, and $\text{B}(\text{N}_3)_4^-$, and have studied the combination of N_5^+ with some of these anions. Most of these compounds are extremely energetic and shock sensitive.

We have studied the reactions of the NF_4^+ and N_2F_3^+ cations with HN_3 in HF solution. The synthesis of the N_7^- anion was also pursued by preparing and characterizing R_3SiNCl_2 and $(\text{R}_3\text{Si})_2\text{NCl}$ compounds. Although their chlorine atoms could not be replaced by azido groups, the reaction of the latter with HF/MF₅ resulted in the isolation of salts of the novel monochloroammonium cation.

Enthalpies of formation were calculated for gas phase N_3 , N_3^- , N_5^+ , and N_5^- from *ab initio* molecular orbital theory. Stability calculations were carried out for solid N_5^+N_3^- and N_5^+N_5^- , using these values and lattice energy estimates.

The possible existence of FN_5 was studied both experimentally by FT-IR spectroscopy of the volatile decomposition products from the thermolysis of $(\text{N}_5^+)_2\text{SnF}_6^{2-}$ and computationally using a RRKM analysis.